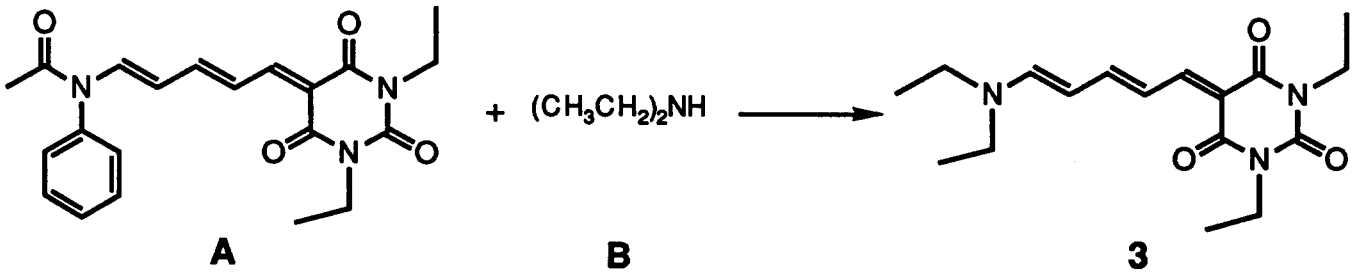
J-2620-M1

Synthesis of 1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene) barbituric acid, **3**.



A **B** **3**

The synthesis of the starting material 1,3-diethyl-5-(5-acetanilidopenta-2,4-dienylidene) barbituric acid, **A**, has been reported previously.[9] 1.3g (3.41 mmol) of **A** was dissolved in 25ml of methylene chloride. While gently warming the solution, 0.9ml (8.72 mmol) of diethylamine was added with swirling, causing an immediate color change to magenta. Excess diethylamine and methylene chloride were removed under reduced pressure, resulting in an inky oil with a metallic greenish sheen. The oil was redissolved in 10ml of fresh methylene chloride. Diethyl ether (100 ml) was added dropwise, resulting in crystal precipitation. The crystals were filtered, washed with ether and dried in air. Yield 0.950 g (87%).

Characterizing data for **3**: ^{1}H NMR. δ 8.00 (d, J = 13.3 Hz, 1H), 7.72 (dd, J = 13.3, 13.2 Hz, 1H), 7.26 (dd, J = 13.2, 12.2 Hz, 1H), 7.05 (d, J = 12.3 Hz, 1H), 5.68 (dd, J = 12.3, 12.2 Hz, 1H), 4.00 (q, J = 7.0 Hz, 4H), 3.37 (m, 4H), 1.27 (m, 6H), 1.23 (t, J = 7.0 Hz, 3H), 1.22 (t, J = 7.0 Hz, 3H). Elemental Analysis: Calculated for $C_{17}H_{25}N_3O_3$: C, 63.93; H, 7.89; N, 13.16; Found: C, 63.92; H, 7.91; N, 13.19.

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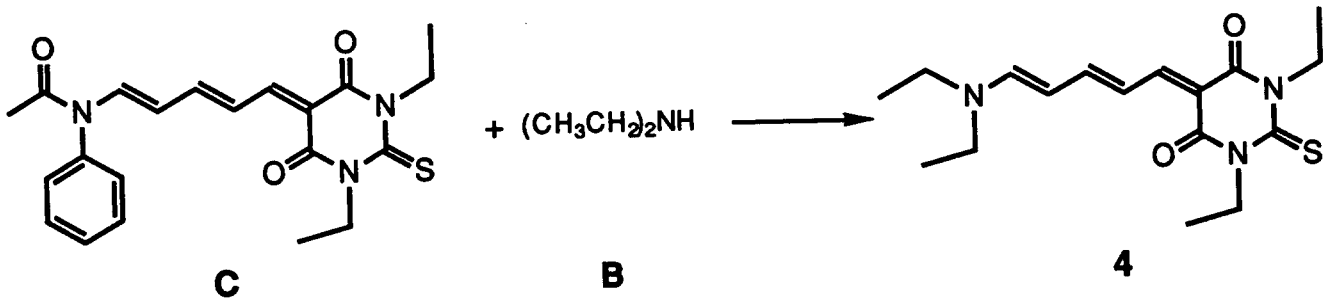
J-2620-M2

Synthesis of 1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid, **4**.



C **B** **4**

The synthesis of the starting material 1,3-diethyl-5-(5-acetanilidopenta-2,4-dienylidene)-2-thiobarbituric acid, **C**, has been reported previously.[9] 1.3g (3.27 mmol) of **C** was dissolved in 25ml of methylene chloride. While gently warming the solution, 0.9ml (8.72 mmol) of diethylamine was added with swirling, causing an immediate color change to magenta. Excess diethylamine and methylene chloride were removed under reduced pressure, resulting in an inky oil with metallic greenish-gold sheen. The oil was redissolved in 10ml of fresh methylene chloride. Diethyl ether (100 ml) was added dropwise, resulting in crystal precipitation. The crystals were filtered, washed with ether and dried in air. Yield 0.920 g (84%).

Characterizing data for **4**: ^{1}H NMR. δ 7.99 (d, J = 13.5 Hz, 1H), 7.79 (dd, J = 13.5, 12.3 Hz, 1H), 7.33 (dd, J = 12.4, 13.0 Hz, 1H), 7.18 (d, J = 12.2 Hz, 1H), 5.79 (dd, J = 12.2, 12.4 Hz, 1H), 4.57 (q, J = 6.9 Hz, 4H), 3.42 (q, J = 7.1 Hz, 4H), 1.30 (m, 12H). Elemental Analysis: Calculated for $C_{17}H_{25}N_3O_2S$: C, 60.87; H, 7.51; N, 12.53; S, 9.56. Found: C, 60.77; H, 7.56; N, 12.44; S, 9.63.

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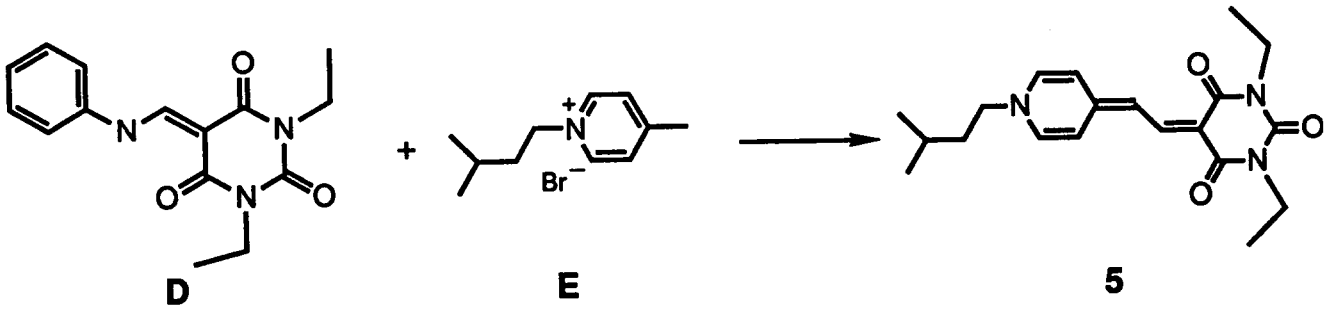
J-2620-M3

Synthesis of 1,3-diethyl-5-[(1-isopentyl-4-pyridylidene)-ethylene]-barbituric acid, **5**.



D **E** **5**

The synthesis of the starting material 1,3-diethyl-5-anilinylidene barbituric acid, **D**, has been reported previously.[9] 3.97g (16.2 mmol) of isopentyl-4-picolinium bromide, **E**, and 4.9g (17.1 mmol) of **D** were added to 50ml toluene while gently heating the solution. Then, 2.5ml of triethylamine was added and the reaction mixture refluxed for 2.5 hours at 110°C. Toluene was removed under vacuum and water was added to the remaining residue. An orange precipitate formed upon addition of the water. This precipitate was dissolved in toluene and dichloromethane and separated from the water layer. The solution was dried over Magnesium Sulfate, filtered and the remaining solvent removed under vacuum. The residue was recrystallized from toluene. Yield 1.98g (34.2%).

Characterizing data for 5: ^{1}H NMR. δ 8.38 (d, J = 15.0 Hz, 1H), 7.36 (d, J = 14.8 Hz, 1H), 7.36 (d, J = 7.2 Hz, 2H), 7.6 - 7.0 (very broad peak, due to hindered rotation, 2H), 4.00 (q, J = 7.0 Hz, 4H), 3.90 (m, 2H), 1.72 (m, 2H), 1.67 (m, 1H), 1.22 (t, J = 6.9 Hz, 6H), 0.98 (d, J = 6.6, 6H). Elemental Analysis: Calculated. for $C_{20}H_{27}N_3O_3$: C, 67.20; H, 7.61; N, 11.76; Found: C, 67.32; H, 7.60; N, 11.76.

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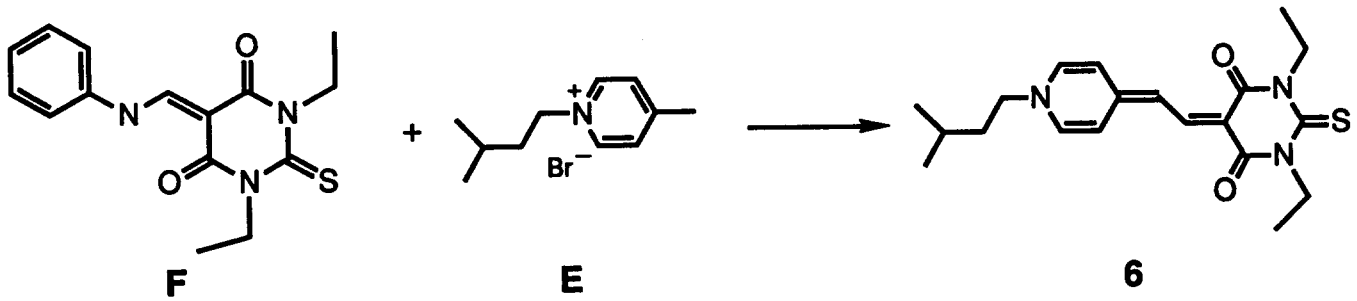
J-2620-M4

Synthesis of 1,3-diethyl-5-[(1-isopentyl-4-pyridylidene)-ethylene]-2-thiobarbituric acid, **6**.



F **E** **6**

The synthesis of the starting material 1,3-diethyl-5-anilinylidene-2-thiobarbituric acid, **F**, has been reported previously.[9] 3.60g (14.8 mmol) of isopentyl-4-picolinium bromide, **E**, and 4.48g (14.8 mmol) of **F** were added to 50ml toluene while gently heating the solution. Then, 2.5ml of triethylamine was added and the reaction mixture refluxed for 2 hours at 110°C. Toluene was removed under vacuum and water was added to the remaining residue. A red precipitate formed upon addition of the water. This precipitate was dissolved in toluene and dichloromethane and separated from the water layer. The solution was dried over Magnesium Sulfate, filtered and the remaining solvent removed under vacuum. The residue was recrystallized from toluene to give red crystals. Yield 2.43g (44%).

Characterizing data for **6**: ^{1}H NMR. δ 8.36 (d, J = 15.3 Hz, 1H), 7.64 (d, J = 15.1 Hz, 1H), 7.49 (d, J = 7.3 Hz, 2H), 7.34 (broad peak, due to hindered rotation, 2H), 4.60 (q, J = 6.9 Hz, 4H), 3.98 (m, 2H), 1.75 (m, 2H), 1.63 (m, 1H), 1.31 (t, J = 6.9 Hz, 6H), 0.99 (d, J = 6.7, 6H). Elemental Analysis: Calculated. for $C_{20}H_{27}N_3O_2S$: C, 64.31; H, 7.29; N, 11.25; S, 8.58; Found: C, 64.21; H, 7.26; N, 11.28; S, 8.50.

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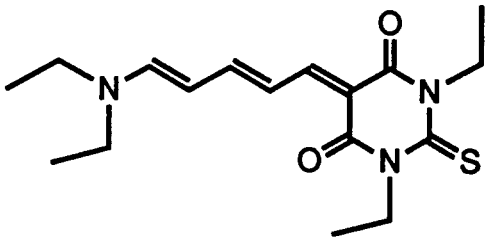
X-RAY CRYSTALLOGRAPHIC SUPPLEMENTARY MATERIAL FOR COMPOUND 4



1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid

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J-2620-M6

Name	1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid
Formula	$C_{17}H_{25}N_3O_2S$
Formula Weight	335.46
Crystal System	triclinic
Space Group	$P\bar{1}$
Cell Dimensions a, Å	10.272 (2)
b, Å	10.288 (1)
c, Å	10.291 (2)
α, °	60.97 (1)
β, °	87.03 (1)
γ, °	70.57 (1)
V, $Å^3$	888.8 (3)
Z	2
Density, calc, g cm^{-3}	1.26
Crystal color, habit	red, irregular prism
Crystal size, mm^3	0.33 x 0.35 x 0.56
μ, cm^{-1}	1.86
μ r_{max}	0.71073
maximum 2θ (scan type)	28°
range of h,k, l	-13-13, -13-13, -13-13
# of reflections measured	8687
# of independent reflections	4292
# reflections, $F_o^2 > 0$	3973
# reflections, $F_o^2 > 3\sigma(F_o^2)$	3326
GOF, merge	1.01
R(merge) for refs meas. twice	0.019
secondary extinction (x 10^{-6})	2.16(29)
R, $F_o^2 > 0$	0.046
R, $F_o^2 > 3\sigma (F_o^2)$	0.038
GOF (number of parameters)	2.34, (309)
$(\Delta/\sigma)_{max}$ in final least squares	<0.005
Final Difference map:	
Maximum, $eÅ^{-3}$	+ 0.34
Minimum, $eÅ^{-3}$	- 0..28

Data were collected at 296 K.
Hydrogen positions were assumed, C-H 0.95 Å, and repositioned once near the end of refinement.
Structure solved using MULTAN 88.

J-2620-177

X-ray I.D. SRM31

Name of Compound Diethylamino-II-Thiobarbituric Acid

Chemical Formula $C_{17}H_{25}N_3O_2S$ M. wt. 335.46

Crystal System Triclinic Space Group $P\bar{1}$ (# 2

a=	10.272(2)	Å	α=	60.97(1)°	
b=	10.288(1)	Å	β=	87.03(1)°	
c=	10.291(2)	Å	γ=	70.57(1)°	
V=	888.8(3)	Å^3	Z=	2	
D_m	—	g cm^{-3}	D_x	1.26	g cm^{-3}

Radiation used MoKα Wavelength 0.71073 Å

Absorption Coefficient, μ= 1.86 cm^{-1} Temperature 296 °K

Type of Absorption Correction none (program used) —

Range of Transmission Factors —

Crystal Color red Crystal Shape (Habit) irregular prism

Crystal Size 0.33 mm × 0.35 mm × 0.56 mm

Source of Crystal synthesized by BGT

Type of Diffractometer Enraf-Nonius Cad-4

Data Collection method (diffraction geometry, scan type) θ-2θ scans

Lattice Parameters: Number of reflections 25 ; θ range 4° to 16°

θ range for data collection 1° to 28°

h_{min} -13 h_{max} 13 k_{min} -13 k_{max} 13 l_{min} -13 l_{max} 13

Number of reflections measured 8687

Number of independent reflections 4292

Number of reflections used in refinement 4292

Criterion for reflections used all used, F_o^2 positive and negative

Goodness of fit for merging data 1.01 (number of multiples 4292)

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R_{int} for duplicate reflections 0.019 (number of duplicates 3815)

Number of standard reflections 3 Interval 150 minutes

Variations of standards within counting statistics

How structure solved? Sharpened Patterson map gave vectors which were interpreted to give positions of ring atoms and the sin connected to them; remaining atoms found from subsequent Structure Factor - Fourier calculation.

How H atoms treated? all refined with isotropic displacement parameters

Refinement on F^2, $w=1/\sigma^2(F_o^2)$, one full matrix used.

R = 0.046 on F for 3973 reflections with $F_o^2 > 0$

R = 0.038 on F for 3326 reflections with $F_o^2 > 3\sigma(F_o^2)$

wR = 0.008 on F^2 for 4292 reflections

Goodness of Fit (S) = 2.34 for 4292 data and 309 parameters

$(\Delta/\sigma)_{max}$ in final least squares cycle < 0.005

$\Delta\rho_{max}$ +0.34 eÅ^{-3}, $\Delta\rho_{min}$ −0.28 eÅ^{-3} in final difference map.

Secondary Extinction parameter (if used) 2.16 (29) $\times 10^{-6}$

(Reference: Larson, A. C. (1967). *Acta Cryst.* 23, 644-665.)

Computer Programs

The CRYM Crystallographic Computing System

(Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14, p. 29.)

ORTEP

(Johnson, C. K. (1976). *ORTEP*II. Report ORNL-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.)

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MULTAN88

Debaerdemaeker, T., Germain, G., Main, P., Refaat, L. S., Tate, C. & Woolfson, M. M. (1988). *MULTAN 88. Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*, Univs. of York, England and Louvain, Belgium.

Scattering Factors and f', f'':

Cromer, D. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Any additional Data:

Structure solved and refined by R. E. Marsh.

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \frac{\Sigma w(F_o^2 - F_c^2)^2}{\Sigma w(F_o^2)^2}$$

$$S = \left\{\frac{\Sigma w(F_o^2 - F_c^2)^2}{n-p}\right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

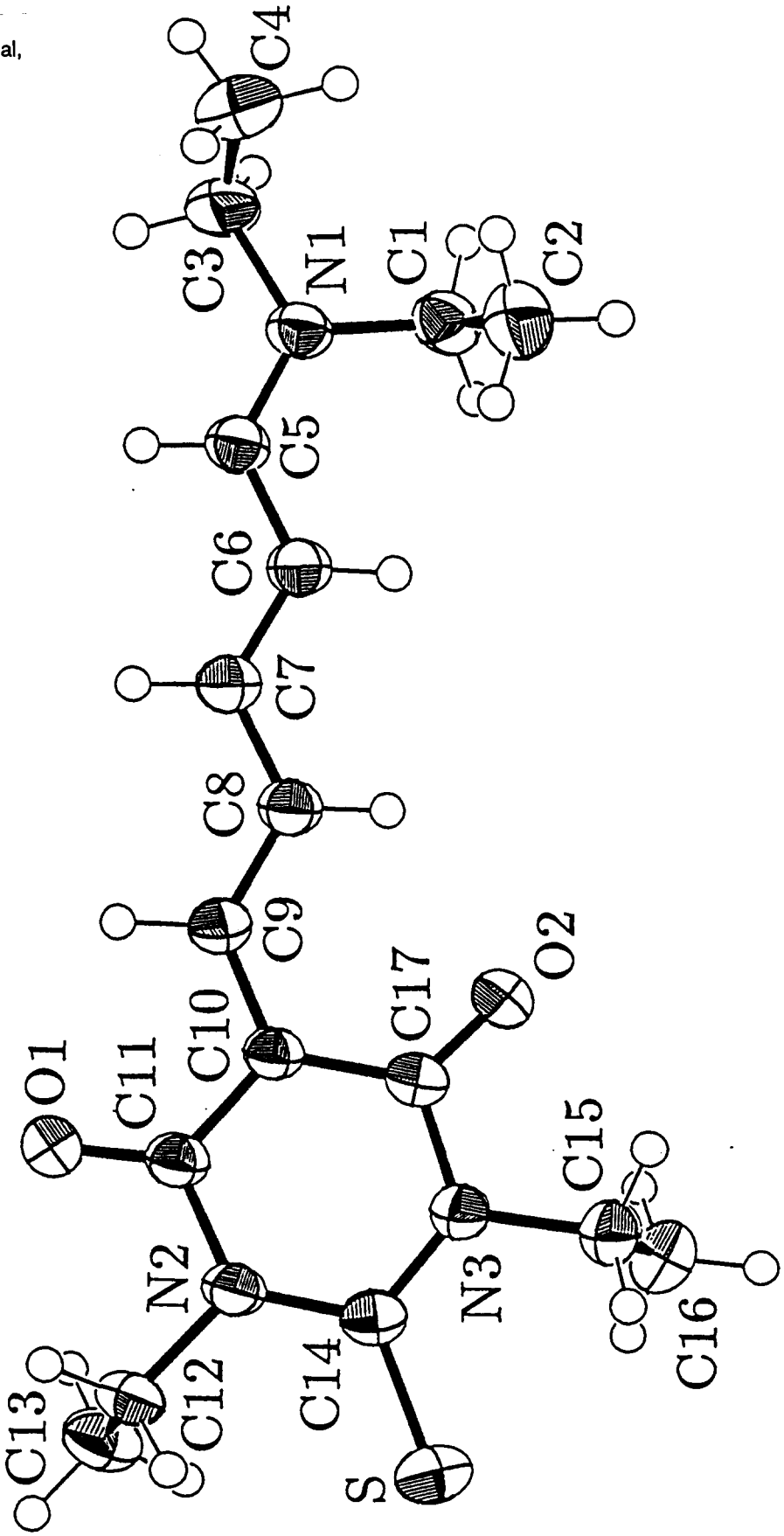
J-2620-MM10

Legends for Figures.

Figure 1. An ORTEP drawing of the molecule with 50 % probability ellipsoids showing the numbering system. Hydrogen atoms are shown with arbitrary, small displacement parameters.

Figure 2. An ORTEP drawing of the contents of a unit cell with a unit cell outlined. Atoms are shown as 50 % probability ellipsoids; hydrogen atoms are as in Fig. 1. The view is perpendicular to the a c plane.

J-2620-M11



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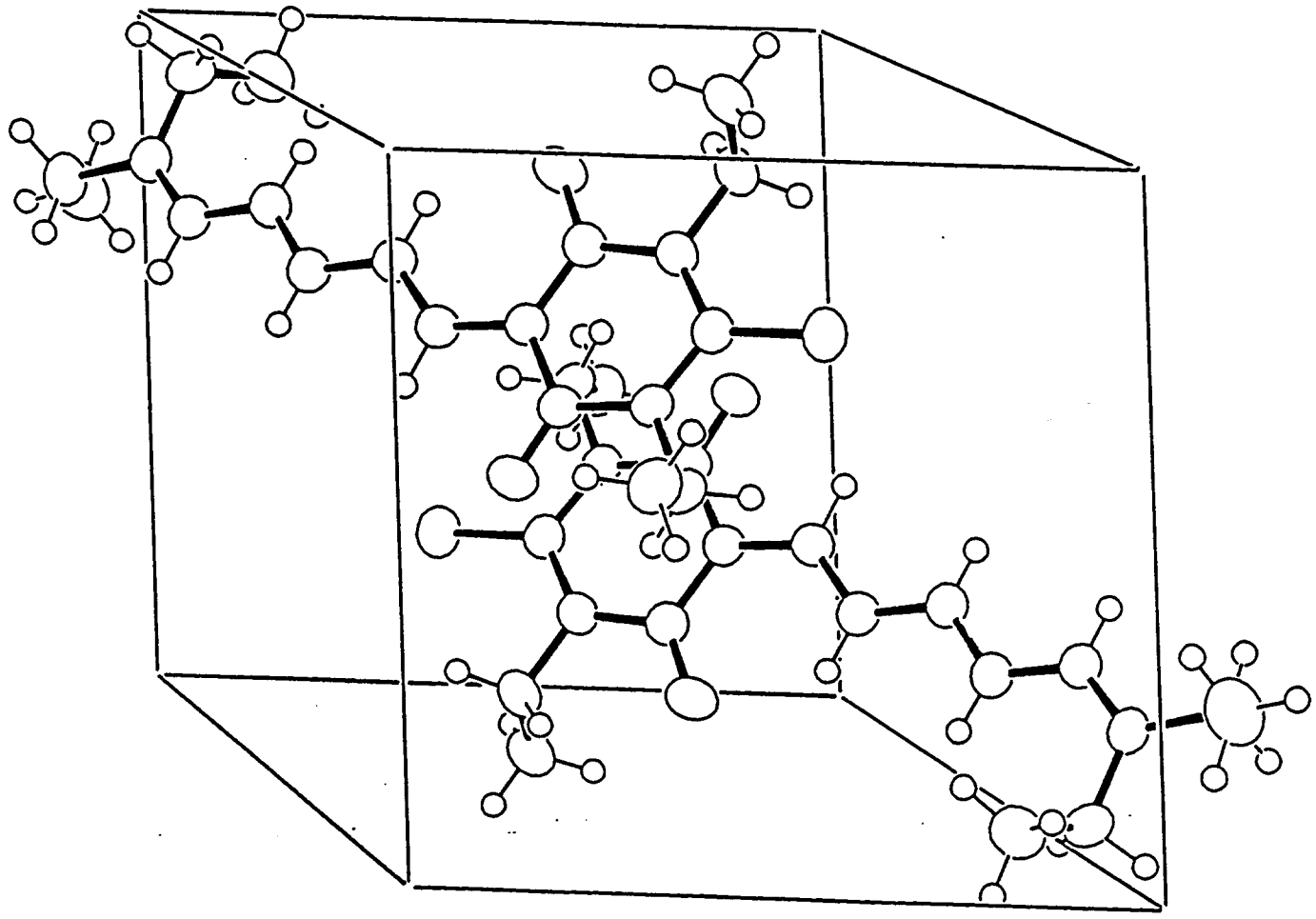
J-2620-M12



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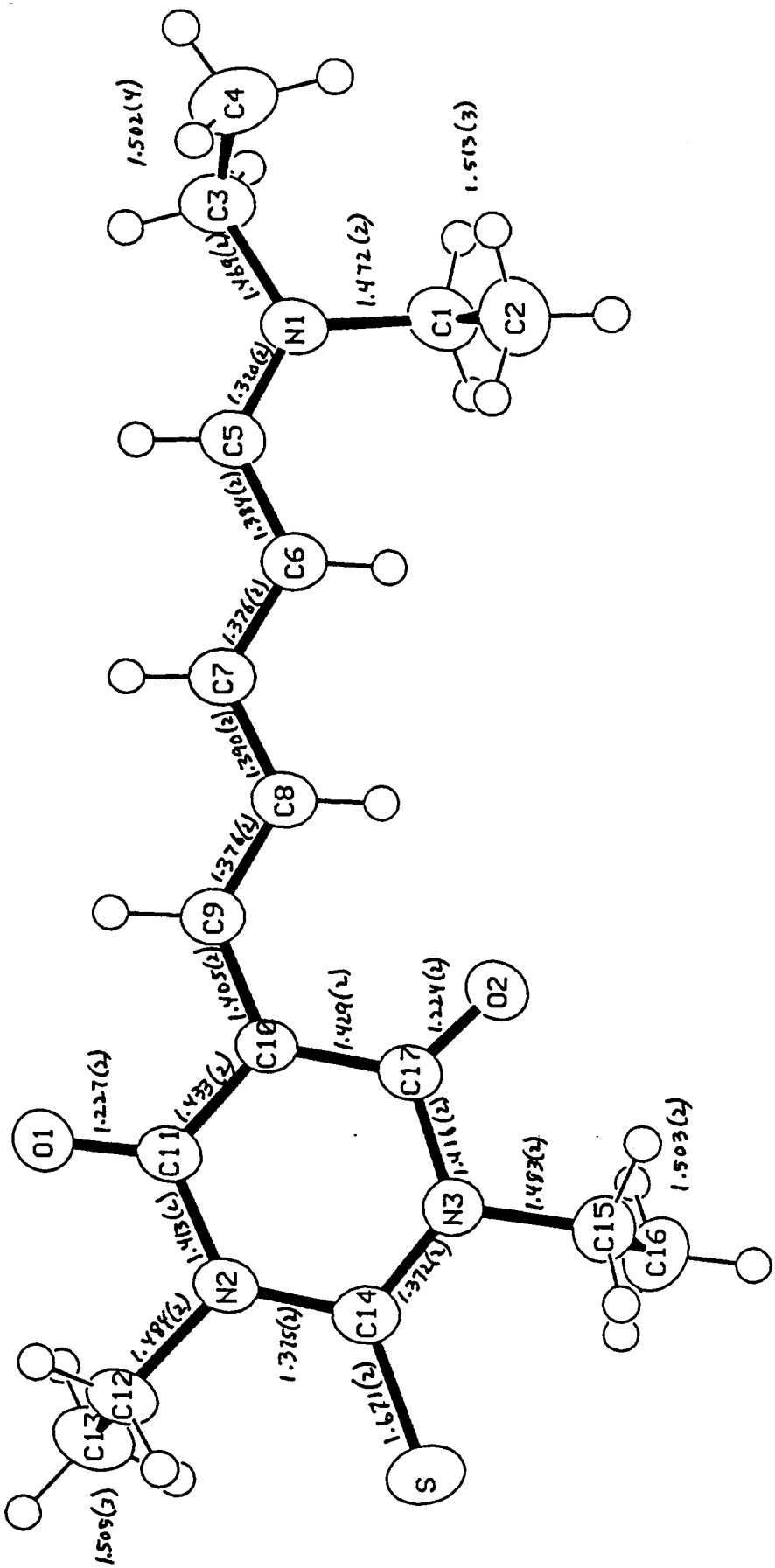
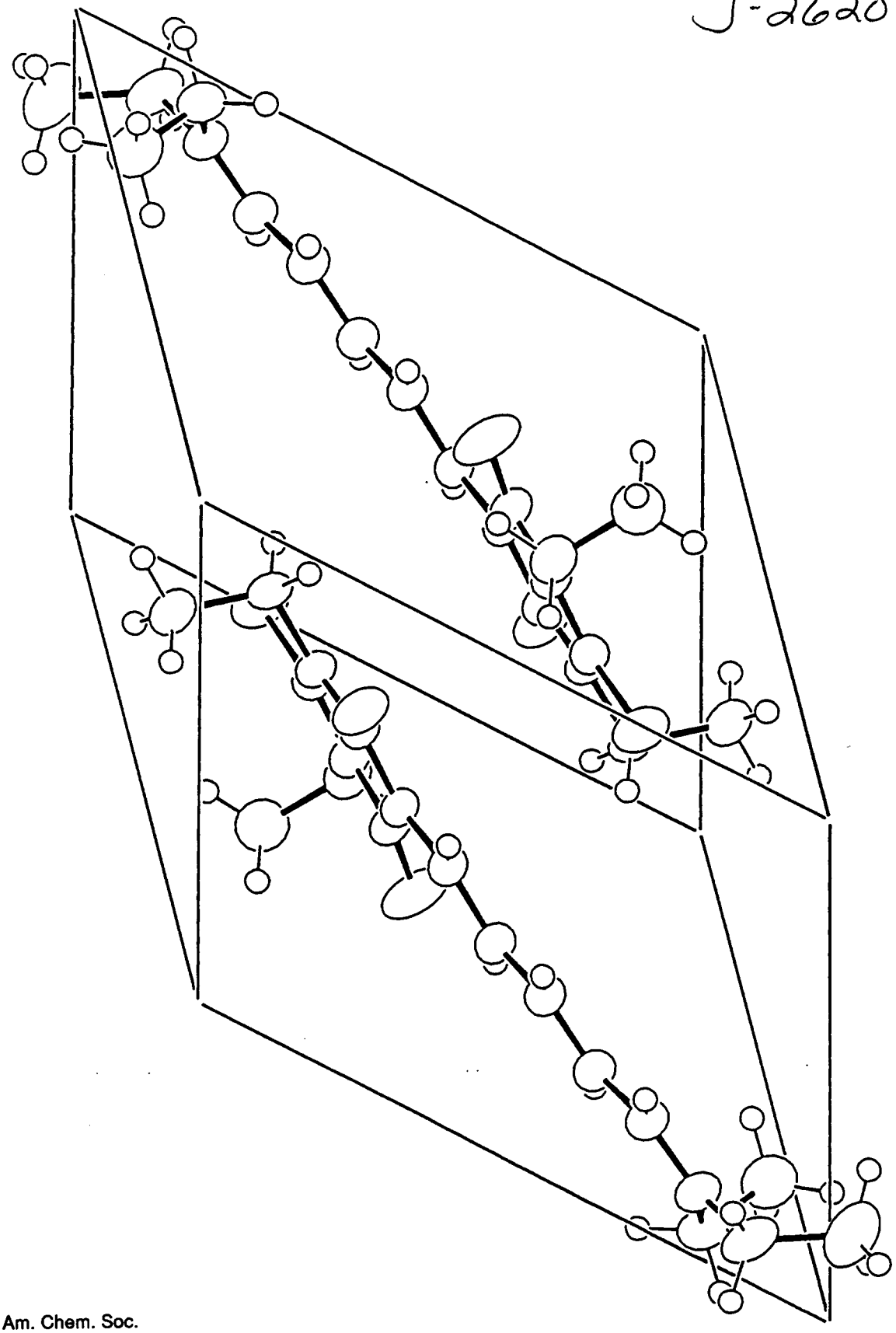
J-2620-M13



J-2620-M14



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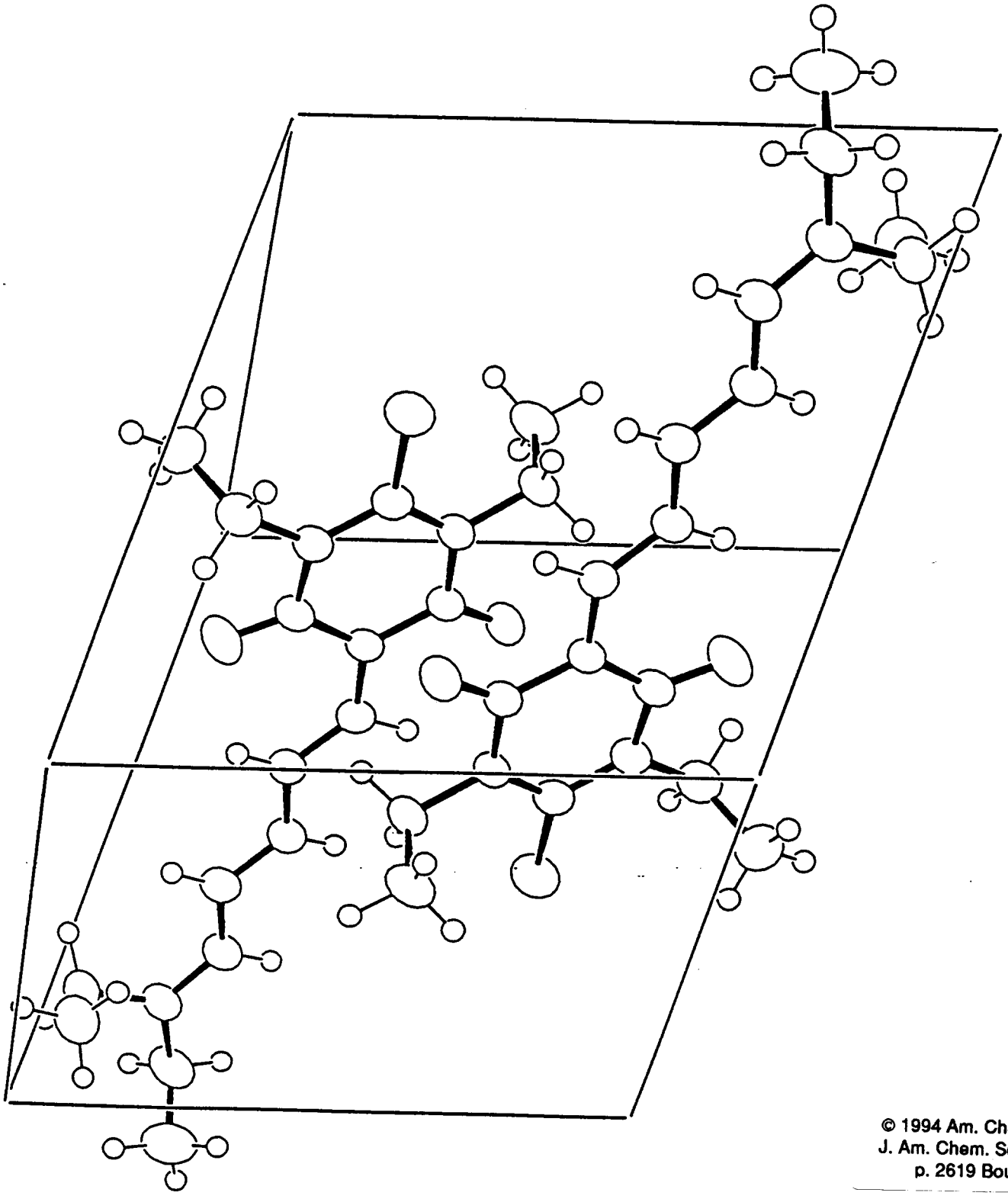
J-2620-MS



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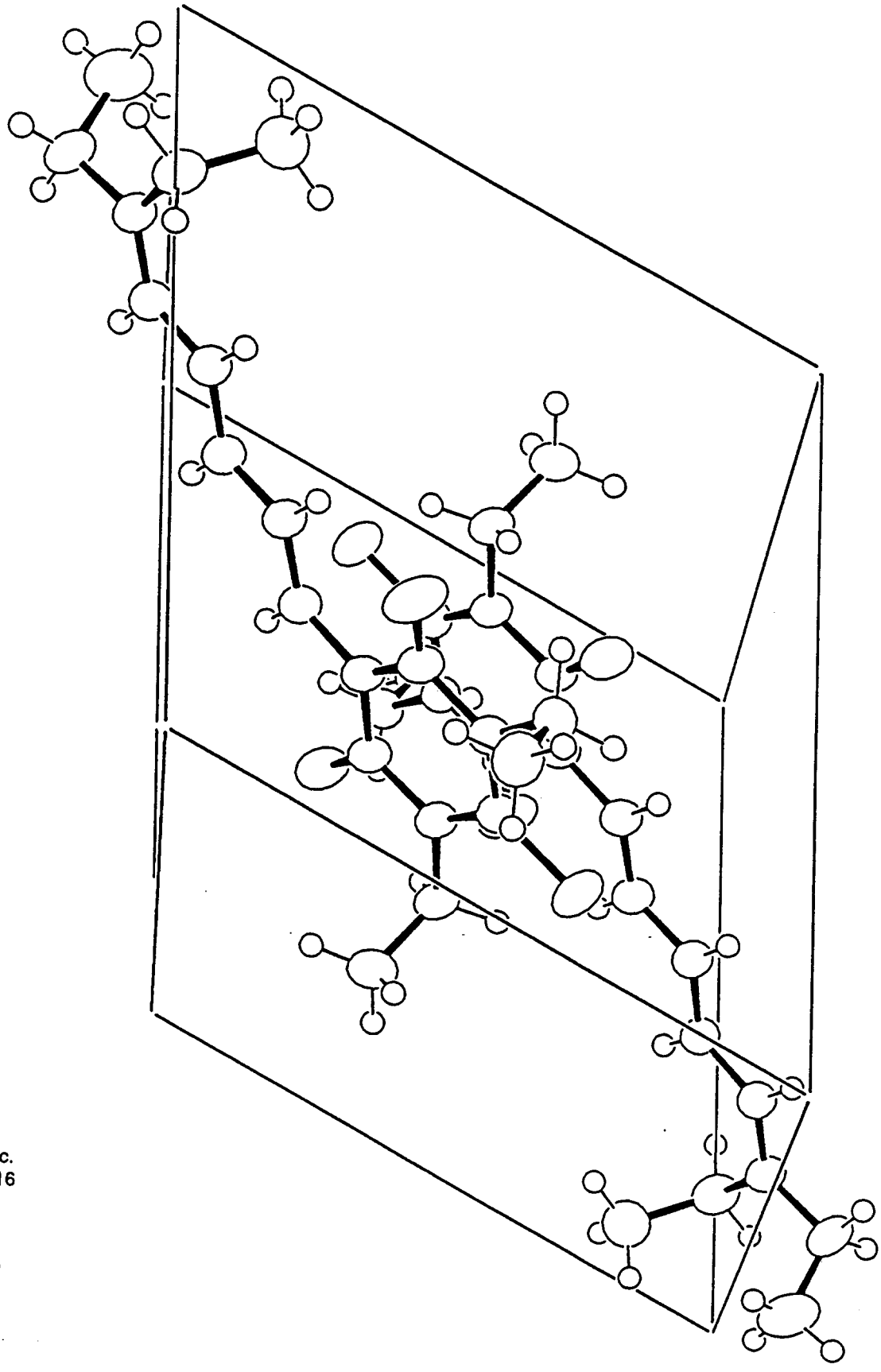
J-2620-M16



J 2620-M17

Table 1. Final Parameters for Diethylamino-II-Thiobarbituric Acid.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq} or B
N1	1804(1)	2209(1)	−602(1)	426(3)
C1	537(2)	2000(2)	70(2)	494(3)
C2	820(2)	621(2)	1657(2)	626(5)
C3	2260(2)	1608(2)	−1647(2)	581(4)
C4	2763(3)	−172(3)	−894(3)	804(6)
C5	2481(2)	2953(2)	−322(2)	405(3)
C6	2138(2)	3589(2)	618(2)	407(3)
C7	2908(2)	4327(2)	880(2)	408(3)
C8	2597(1)	4920(2)	1863(2)	400(3)
C9	3381(1)	5613(2)	2176(1)	382(3)
C10	3191(1)	6172(1)	3201(1)	361(3)
C11	4195(1)	6775(1)	3394(1)	374(3)
O1	5176(1)	6912(1)	2669(1)	540(2)
N2	4027(1)	7247(1)	4491(1)	370(2)
C12	5032(2)	7956(2)	4597(2)	434(3)
C13	4534(2)	9716(2)	3519(2)	555(4)
C14	2990(1)	7132(1)	5397(1)	381(3)
S	2876(.4)	7680(.5)	6697(.5)	589(1)
N3	2040(1)	6566(1)	5167(1)	385(2)
C15	881(2)	6410(2)	6085(2)	468(3)

J-2620-M18

Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
C16	−396(2)	7887(2)	5390(2)	563(4)
C17	2044(1)	6140(2)	4049(2)	415(3)
O2	1068(1)	5782(2)	3876(1)	683(3)
H1A	26(16)	1858(17)	−612(17)	4.7(3)*
H1B	−37(17)	3036(20)	7(17)	5.0(4)*
H2A	−52(22)	593(22)	2024(22)	7.5(5)*
H2B	1261(19)	−372(23)	1636(20)	6.4(5)*
H2C	1366(18)	766(20)	2293(19)	5.7(4)*
H3A	1473(19)	2073(20)	−2414(19)	5.9(4)*
H3B	2980(18)	1968(20)	−2081(18)	5.4(4)*
H4A	3037(22)	−457(25)	−1598(25)	8.3(6)*
H4B	3605(23)	−595(25)	−158(24)	7.8(6)*
H4C	1962(22)	−524(24)	−433(23)	7.8(5)*
H5	3265(15)	3082(16)	−797(15)	3.4(3)*
H6	1366(15)	3483(16)	1141(15)	3.5(3)*
H7	3672(16)	4468(16)	388(16)	3.8(3)*
H8	1794(15)	4818(15)	2362(15)	3.4(3)*
H9	4209(16)	5710(16)	1666(15)	4.0(3)*
H12A	5155(14)	7689(16)	5619(16)	3.9(3)*
H12B	5936(15)	7383(16)	4392(15)	3.8(3)*

J-2620-M19

Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
H13A	5243(17)	10188(19)	3583(17)	5.4(4)*
H13B	4385(16)	9946(18)	2499(19)	4.8(4)*
H13C	3676(18)	10261(19)	3812(18)	5.2(4)*
H15A	693(16)	5504(18)	6148(17)	4.8(4)*
H15B	1254(15)	6150(17)	7048(16)	4.0(3)*
H16A	−1145(20)	7736(21)	6008(20)	6.5(4)*
H16B	−234(18)	8779(22)	5335(20)	6.4(5)*
H16C	−719(19)	8160(22)	4398(22)	7.0(5)*

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

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Table 2. Anisotropic Displacement Parameters for Diethylamino-II-Thiobarbituric Acid.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N1	506(7)	470(7)	409(6)	−233(5)	66(5)	−258(5)
C1	424(8)	571(9)	580(9)	−199(7)	26(7)	−336(8)
C2	676(12)	695(12)	615(11)	−366(10)	202(9)	−336(10)
C3	743(11)	776(12)	560(10)	−430(10)	195(9)	−484(9)
C4	954(17)	832(14)	1013(17)	−407(13)	375(15)	−706(14)
C5	467(8)	421(7)	388(7)	−201(6)	63(6)	−217(6)
C6	470(8)	403(7)	396(7)	−177(6)	67(6)	−220(6)
C7	448(8)	401(7)	416(7)	−158(6)	54(6)	−228(6)
C8	430(7)	391(7)	436(7)	−157(6)	53(6)	−238(6)
C9	398(7)	366(7)	424(7)	−138(6)	67(6)	−226(6)
C10	378(7)	346(6)	418(7)	−140(5)	55(5)	−226(6)
C11	388(7)	361(7)	430(7)	−145(6)	53(6)	−229(6)
O1	514(6)	748(7)	688(7)	−382(5)	258(5)	−513(6)
N2	382(6)	377(6)	422(6)	−157(5)	37(5)	−233(5)
C12	450(8)	475(8)	486(8)	−211(7)	16(6)	−284(7)
C13	690(11)	481(9)	587(10)	−300(8)	49(8)	−270(8)
C14	427(7)	341(7)	375(7)	−116(6)	25(6)	−188(6)
S	657(3)	779(3)	596(3)	−299(2)	139(2)	−511(2)
N3	438(6)	388(6)	400(6)	−186(5)	102(5)	−226(5)
C15	571(9)	504(9)	429(8)	−289(7)	190(7)	−253(7)
C16	534(9)	658(11)	570(10)	−220(8)	201(8)	−364(9)
C17	457(7)	431(7)	482(8)	−211(6)	104(6)	−288(7)
O2	627(7)	1116(10)	937(9)	−594(7)	403(6)	−816(8)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table 3. Complete Distances and Angles for Diethylamino-II-Thiobarbituric Acid.

	Distance(Å)		Distance(Å)
N1 –C1	1.472(2)	C7 –H7	0.925(16)
N1 –C3	1.469(2)	C8 –H8	0.957(15)
N1 –C5	1.320(2)	C9 –H9	0.984(16)
C1 –C2	1.513(3)	C12 –H12A	0.953(16)
C3 –C4	1.502(4)	C12 –H12B	0.995(16)
C5 –C6	1.384(2)	C13 –H13A	1.021(18)
C6 –C7	1.376(2)	C13 –H13B	0.965(18)
C7 –C8	1.390(2)	C13 –H13C	0.995(19)
C8 –C9	1.376(2)	C15 –H15A	0.985(17)
C9 –C10	1.405(2)	C15 –H15B	0.956(16)
C10 –C11	1.433(2)	C16 –H16A	0.98(2)
C10 –C17	1.429(2)	C16 –H16B	0.96(2)
C11 –O1	1.227(2)	C16 –H16C	0.96(2)
C11 –N2	1.413(2)		
N2 –C12	1.484(2)		
N2 –C14	1.375(2)		
C12 –C13	1.505(3)		
C14 –S	1.671(2)		
C14 –N3	1.372(2)		
N3 –C15	1.483(2)		
N3 –C17	1.416(2)		
C15 –C16	1.503(3)		
C17 –O2	1.224(2)		
C1 –H1A	0.989(17)		
C1 –H1B	1.003(18)		
C2 –H2A	0.96(2)		
C2 –H2B	0.98(2)		
C2 –H2C	0.976(19)		
C3 –H3A	0.97(2)		
C3 –H3B	0.933(19)		
C4 –H4A	0.91(3)		
C4 –H4B	1.00(3)		
C4 –H4C	1.01(2)		
C5 –H5	0.934(16)		
C6 –H6	0.941(16)		

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Table 3. (Cont.)

	Angle(°)		Angle(°)
C3 –N1 –C1	117.4(1)	H2A –C2 –C1	108.7(14)
C5 –N1 –C1	121.6(1)	H2B –C2 –C1	108.8(13)
C5 –N1 –C3	121.0(1)	H2C –C2 –C1	109.6(11)
C2 –C1 –N1	113.9(2)	H2B –C2 –H2A	106.1(18)
C4 –C3 –N1	113.0(2)	H2C –C2 –H2A	109.4(18)
C6 –C5 –N1	126.2(1)	H2C –C2 –H2B	114.1(17)
C7 –C6 –C5	123.1(1)	H3A –C3 –N1	107.4(12)
C8 –C7 –C6	123.3(1)	H3B –C3 –N1	106.7(12)
C9 –C8 –C7	124.1(1)	H3A –C3 –C4	110.1(12)
C10 –C9 –C8	128.3(1)	H3B –C3 –C4	109.8(12)
C11 –C10 –C9	118.2(1)	H3B –C3 –H3A	109.8(17)
C17 –C10 –C9	121.9(1)	H4A –C4 –C3	108.2(16)
C17 –C10 –C11	120.0(1)	H4B –C4 –C3	107.3(14)
O1 –C11 –C10	124.4(1)	H4C –C4 –C3	107.9(14)
N2 –C11 –C10	117.1(1)	H4B –C4 –H4A	107.9(21)
N2 –C11 –O1	118.4(1)	H4C –C4 –H4A	110.7(21)
C12 –N2 –C11	115.7(1)	H4C –C4 –H4B	114.7(20)
C14 –N2 –C11	124.4(1)	H5 –C5 –N1	118.5(10)
C14 –N2 –C12	119.9(1)	H5 –C5 –C6	115.3(10)
C13 –C12 –N2	111.3(1)	H6 –C6 –C5	119.3(10)
S –C14 –N2	121.7(1)	H6 –C6 –C7	117.6(10)
N3 –C14 –N2	116.7(1)	H7 –C7 –C6	120.9(10)
N3 –C14 –S	121.6(1)	H7 –C7 –C8	115.8(10)
C15 –N3 –C14	120.5(1)	H8 –C8 –C7	117.4(9)
C17 –N3 –C14	124.5(1)	H8 –C8 –C9	118.5(9)
C17 –N3 –C15	115.0(1)	H9 –C9 –C8	118.3(10)
C16 –C15 –N3	112.3(1)	H9 –C9 –C10	113.4(9)
N3 –C17 –C10	117.0(1)	H12A –C12 –N2	106.3(10)
O2 –C17 –C10	125.1(1)	H12B –C12 –N2	106.4(9)
O2 –C17 –N3	117.9(1)	H12A –C12 –C13	113.4(10)
H1A –C1 –N1	105.2(10)	H12B –C12 –C13	112.2(9)
H1B –C1 –N1	106.6(10)	H12B –C12 –H12A	106.9(13)
H1A –C1 –C2	111.4(10)	H13A –C13 –C12	110.7(10)
H1B –C1 –C2	112.0(11)	H13B –C13 –C12	111.2(11)
H1B –C1 –H1A	107.3(14)	H13C –C13 –C12	109.9(11)

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Table 3. (Cont.)

	Angle(°)
H13B –C13 –H13A	108.5(15)
H13C –C13 –H13A	104.8(15)
H13C –C13 –H13B	111.6(15)
H15A –C15 –N3	104.9(10)
H15B –C15 –N3	104.9(10)
H15A –C15 –C16	110.8(10)
H15B –C15 –C16	113.2(10)
H15B –C15 –H15A	110.4(14)
H16A –C16 –C15	110.2(12)
H16B –C16 –C15	111.9(12)
H16C –C16 –C15	111.6(13)
H16B –C16 –H16A	105.8(18)
H16C –C16 –H16A	108.6(18)
H16C –C16 –H16B	108.6(18)

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Table 4. Intermolecular Distances Less than 3.5 Å for Diethylamino-II-Thiobarbituric Acid.

	Distance(Å)		Distance(Å)
C1 –C8	3.481(2)	C8 –H1A	3.191(17)
C3 –O1	3.344(2)	C8 –H1B	2.822(18)
C5 –O1	3.307(2)	C8 –H16A	3.32(2)
C9 –C12	3.452(2)	C8 –H12A	3.000(16)
C10 –N2	3.477(2)	C8 –H12B	3.479(16)
C11 –C11	3.440(2)	C9 –H4C	3.37(2)
C11 –N2	3.441(2)	C9 –H1A	3.474(17)
O1 –C14	3.458(2)	C9 –H12A	2.903(16)
O1 –N3	3.473(2)	C9 –H12B	3.274(16)
C15 –O2	3.465(2)	C10 –H2B	3.04(2)
O2 –O2	3.312(2)	C10 –H12A	3.345(16)
C1 –H8	3.189(15)	C10 –H12B	3.094(16)
N1 –H13B	3.493(18)	C11 –H2B	3.24(2)
N1 –H15A	3.286(17)	C11 –H4B	3.25(3)
N1 –H15B	3.422(16)	O1 –H4B	2.85(3)
C1 –H4C	3.31(2)	O1 –H3B	2.437(19)
C2 –H16C	3.48(2)	O1 –H5	2.440(16)
C2 –H4C	3.23(2)	N2 –H2B	3.46(2)
C2 –H16B	3.43(2)	N2 –H2C	3.437(19)
C3 –H15A	3.327(17)	C12 –H3B	3.200(19)
C3 –H16C	3.18(2)	C12 –H13A	3.208(18)
C3 –H12B	3.222(16)	C13 –H2C	3.180(19)
C4 –H2A	3.31(2)	C13 –H3B	3.296(19)
C4 –H13A	3.360(18)	C13 –H4A	3.16(3)
C4 –H13B	3.308(18)	C13 –H12A	3.303(16)
C5 –H13B	3.110(18)	C13 –H13A	3.055(18)
C5 –H15A	3.419(17)	C13 –H13C	3.398(19)
C5 –H15B	2.948(16)	C14 –H2C	3.432(19)
C6 –H13B	3.285(18)	S –H4A	3.21(3)
C6 –H13C	3.323(19)	S –H2A	3.43(2)
C6 –H15B	3.260(16)	S –H9	3.441(16)
C6 –H1B	3.181(18)	S –H16B	3.41(2)
C6 –H16A	3.30(2)	S –H13A	3.283(18)
C7 –H1B	3.074(18)	N3 –H2B	3.36(2)
C7 –H12A	3.462(16)	C15 –H8	3.405(15)

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Table 4. (Cont.)

	Distance(Å)		Distance(Å)
C16 –H2A	3.32(2)	H3A –H12B	3.30(3)
C16 –H3A	3.29(2)	H3B –H15A	3.23(3)
C16 –H2C	3.262(19)	H3B –H16C	3.49(3)
C16 –H6	3.377(16)	H3B –H12B	2.45(3)
C16 –H8	3.349(15)	H3B –H13A	3.31(3)
C16 –H16B	3.42(2)	H3B –H13B	2.92(3)
C17 –H2B	3.06(2)	H4A –H16C	3.15(3)
C17 –H1A	3.474(17)	H4A –H13A	2.60(3)
C17 –H12B	3.117(16)	H4A –H13B	2.89(3)
O2 –H1A	3.018(17)	H4B –H9	3.16(3)
O2 –H3A	2.70(2)	H4B –H13B	3.23(3)
O2 –H15A	2.579(17)	H4B –H5	3.20(3)
O2 –H12B	3.394(16)	H4B –H13B	3.06(3)
H1A –H1A	3.41(2)	H4C –H9	3.38(3)
H1A –H2A	3.46(3)	H5 –H13B	3.25(2)
H1A –H2B	2.87(3)	H5 –H15A	3.46(2)
H1A –H4C	2.72(3)	H5 –H15B	2.91(2)
H1A –H8	2.92(2)	H5 –H9	3.15(2)
H1B –H6	2.98(2)	H6 –H13C	3.28(2)
H1B –H8	2.58(2)	H6 –H6	3.30(2)
H2A –H16B	3.02(3)	H6 –H15B	3.22(2)
H2A –H16C	2.78(3)	H6 –H16A	2.60(3)
H2A –H3A	3.37(3)	H7 –H7	3.19(2)
H2A –H4A	3.18(3)	H7 –H9	2.98(2)
H2A –H4C	2.66(3)	H8 –H15A	2.94(2)
H2A –H16B	3.13(3)	H8 –H16A	2.63(3)
H2B –H16C	3.43(3)	H8 –H12A	3.30(2)
H2B –H4C	3.26(3)	H8 –H12B	3.42(2)
H2C –H13B	2.92(3)	H9 –H12A	3.11(2)
H2C –H13C	2.67(3)	H12A –H13A	2.59(2)
H2C –H16B	3.49(3)	H12A –H13C	3.03(3)
H2C –H16A	2.80(3)	H13A –H13A	2.79(3)
H2C –H16B	2.83(3)	H13A –H13C	2.72(3)
H3A –H15A	2.91(3)	H13C –H16A	2.79(3)
H3A –H16C	2.37(3)	H13C –H13C	3.48(3)

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Table 4. (Cont.)

	Distance(Å)
H16B –H16B	2.47(3)

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Table 5. Observed and Calculated Structure Factors for Diethylamino-II-Thiobarbituric Acid

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\sigma F_{obs}$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

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F2620-m28

-12	1	1	
1	18	17	2
2	13	15	2
3	7	3	3
4	27	23	1

-11	1	1	
1	-10	5	2
2	8	3	3
3	27	25	1
4	17	17	2
5	1	0	6
6	18	18	2
7	8	2	3

-11	2	1	
1	17	18	2
2	6	3	4
3	31	32	1
4	54	51	1
5	7	7	3
6	16	14	2

-11	3	1	
1	11	9	2
2	8	13	3
3	-6	1	3
4	7	6	3
5	10	4	3
6	32	31	1

-10	1	1	
1	11	10	2
2	15	17	1
3	13	15	2
4	34	31	1
5	49	50	1
6	-9	4	2
7	19	17	2
8	26	27	1

-10	2	1	
1	10	11	2
2	37	34	1
3	32	35	1
4	24	30	1
5	48	46	1
6	3	4	5
7	-10	3	2
8	13	14	2

-10	3	1	
1	16	18	2
2	-4	3	4
3	32	32	1
4	58	62	1
5	26	29	1
6	9	6	3
7	-2	2	6
8	45	39	1

-10	4	1	
1	9	8	3
2	21	21	1
3	27	28	1
4	29	24	1
5	19	19	2
6	33	35	1
7	15	18	2

-10	5	1	
2	16	13	2
3	52	50	1
4	36	39	1
5	5	4	4

-9	1	1	
1	21	23	1
2	69	66	1
3	15	14	1
4	96	99	1
5	86	91	1
6	49	53	1
7	39	39	1
8	22	22	1
9	13	5	2

-9	2	1	
1	8	13	2
2	25	27	1
3	2	12	5
4	30	26	1
5	5	3	3
6	17	13	1
7	-10	4	2
8	10	9	2
9	77	73	1

-9	3	1	
1	23	18	1
2	31	30	1
3	58	61	1
4	73	73	1
5	43	43	1
6	13	12	2
7	84	83	1
8	6	4	4
9	29	27	1

-9	4	1	
1	17	14	2
2	10	6	2
3	4	0	4
4	50	48	1
5	22	23	1
6	41	37	1
7	30	32	1
8	33	32	1
9	27	23	1

-9	5	1	
1	9	11	3
2	24	23	1
3	11	9	2
4	38	39	1
5	29	27	1
6	-6	6	4
7	32	27	1
8	41	41	1

-9	6	1	
2	13	12	2
3	19	17	2
4	39	38	1
5	42	43	1
6	9	2	3
7	-1	9	6

-8	1	1	
1	-7	9	2
2	37	36	1
3	45	40	1
4	45	54	1
5	82	85	1
6	71	70	1
7	-5	5	3
8	55	54	1
9	20	23	1
10	57	53	1

-8	2	1	
1	32	35	1
2	11	12	2
3	-6	2	2
4	105	108	1
5	122	126	1
6	16	17	1
7	44	44	1
8	55	59	1
9	17	19	2
10	16	12	2

-8	3	1	
1	18	20	1
2	21	21	1
3	61	59	1
4	21	20	1
5	22	19	1
6	7	0	3
7	56	58	1
8	18	19	1
9	46	44	1
10	-8	3	3

-8	4	1	
1	31	33	1
2	23	27	1
3	-3	2	4
4	65	61	1
5	80	81	1
6	53	54	1
7	8	3	3
8	56	53	1
9	12	13	2
10	11	8	2

-8	5	1	
1	15	16	2
2	2	1	5
3	34	30	1
4	23	20	1
5	12	4	2
6	72	75	1
7	16	16	2
8	15	13	2
9	-12	3	2

-8	6	1	
1	12	2	2
2	2	5	5
3	41	39	1
4	20	19	1
5	30	33	1
6	8	1	3
7	64	62	1
8	29	26	1
9	-4	4	4

-8	7	1	
2	24	19	1
3	39	39	1

-7	1	1	
4	52	50	1
5	8	4	3
6	1	5	7
7	-5	4	4
8	17	21	2

-7	1	1	
1	125	126	1
2	71	69	1
3	99	99	1
4	31	33	1
5	8	16	2
6	61	67	1
7	48	45	1
8	43	42	1
9	13	5	2
10	50	47	1

-7	2	1	
1	110	108	1
2	99	101	1
3	103	103	1
4	125	126	1
5	42	46	1
6	79	77	1
7	53	57	1
8	7	13	3
9	39	37	1
10	38	35	1
11	-7	3	3

-7	3	1	
1	52	53	1
2	18	26	1
3	18	21	1
4	42	43	1
5	48	50	1
6	52	52	1
7	86	86	1
8	42	40	1
9	18	15	1
10	16	18	2
11	-11	5	2

-7	4	1	
1	28	33	1
2	71	70	1
3	34	32	1
4	25	22	1
5	64	63	1
6	25	24	1
7	6	7	3
8	97	94	1
9	40	36	1
10	-8	8	3
11	28	26	1

-7	5	1	
1	22	21	1
2	18	19	1
3	16	10	1
4	108	106	1
5	72	73	1
6	64	67	1
7	14	9	2
8	34	31	1
9	3	6	5
10	25	22	1

-7	6	1	
1	27	29	1
2	32	34	1

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Diethylamino-II-Thiobarbituric Acid

3	14	4	2
4	16	14	1
5	100	98	1
6	0	2	7
7	32	31	1
8	36	36	1
9	12	15	2
10	36	34	1

-7 7 1

1	-5	6	4
2	56	56	1
3	15	4	2
4	43	38	1
5	69	69	1
6	19	20	1
7	46	45	1
8	-8	9	3
9	21	20	1

-7 8 1

2	49	48	1
3	42	40	1
4	45	44	1
5	32	31	1
6	0	0	8
7	8	8	3
8	7	2	4

-6 1 1

1	39	35	0
2	115	108	1
3	163	168	1
4	33	33	1
5	32	35	1
6	84	86	1
7	75	72	1
8	90	91	1
9	11	12	2
10	55	55	1
11	12	15	2

-6 2 1

1	207	201	1
2	174	173	1
3	60	63	1
4	5	3	3
5	23	21	1
6	94	97	1
7	20	18	1
8	70	71	1
9	76	75	1
10	-5	6	4
11	-6	9	3

-6 3 1

1	84	78	1
2	25	25	1
3	18	22	1
4	39	38	1
5	92	91	1
6	16	11	1
7	44	43	1
8	92	91	1
9	120	120	1
10	6	12	3
11	16	15	2

-6 4 1

1	43	44	1
2	16	19	1
3	54	56	1
4	48	49	1
5	62	62	1
6	193	195	1
7	33	35	1
8	14	3	2
9	26	27	1
10	24	22	1
11	-10	4	2

-6 5 1

1	41	45	1
2	44	45	1
3	9	2	2
4	15	8	1
5	67	66	1
6	129	129	1
7	19	20	1
8	99	95	1
9	33	34	1
10	12	12	2
11	54	51	1

-6 6 1

1	11	14	2
2	22	24	1
3	128	125	1
4	47	48	1
5	16	3	1
6	26	20	1
7	12	10	2
8	17	17	1
9	17	16	1
10	56	53	1
11	24	23	1

-6 7 1

1	8	7	3
2	-6	2	3
3	46	44	1
4	98	97	1
5	137	137	1
6	51	52	1
7	14	13	2
8	35	36	1
9	-10	0	2
10	14	9	2

-6 8 1

1	10	13	3
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3	12	8	2
4	34	29	1
5	54	53	1
6	40	42	1
7	27	27	1
8	13	8	2
9	58	54	1
10	24	23	1

-6 9 1

3	30	30	1
4	35	33	1
5	42	39	1
6	8	1	3
7	-7	6	3
8	35	33	1

-5 1 1

1	239	232	2
2	202	188	1
3	126	115	1
4	133	135	1
5	-6	4	2
6	9	9	2
7	128	127	1
8	-5	3	3
9	16	13	1
10	78	77	1
11	-9	3	2

-5 2 1

1	16	9	1
2	4	4	2
3	87	81	1
4	127	128	1
5	118	121	1
6	140	142	1
7	158	162	1
8	71	71	1
9	60	59	1
10	20	22	1
11	23	22	1
12	17	17	2

-5 3 1

1	139	138	1
2	84	81	1
3	50	51	0
4	119	116	1
5	89	88	1
6	74	75	1
7	221	223	2
8	21	22	1
9	49	48	1
10	33	33	1
11	54	53	1
12	34	33	1

-5 4 1

1	73	75	1
2	63	64	1
3	59	57	1
4	168	171	1
5	16	11	1
6	95	94	1
7	96	98	1
8	14	14	1
9	53	48	1
10	35	32	1
11	33	33	1
12	34	34	1

-5 5 1

1	61	59	1
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3	43	43	1
4	169	170	1
5	206	207	1
6	160	157	1
7	138	137	1
8	-7	9	2
9	33	32	1
10	7	11	3
11	10	13	2
12	35	32	1

-5 6 1

1	18	17	1
2	14	10	1
3	41	39	1
4	30	33	1
5	146	146	1
6	212	214	2
7	54	54	1
8	-10	5	2
9	-6	1	3
10	51	49	1
11	23	24	1
12	32	29	1

-5 7 1

1	38	38	1
2	51	49	1
3	12	11	2
4	50	45	1
5	31	25	1
6	60	58	1
7	30	34	1
8	41	42	1
9	24	26	1
10	7	7	3
11	27	20	1

-5 8 1

1	19	16	1
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3	5	3	4
4	74	79	1
5	108	109	1
6	75	77	1
7	12	17	2
8	7	15	3
9	31	26	1
10	65	57	1
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-5 9 1

1	10	7	3
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3	7	7	3
4	15	18	2
5	8	22	3
6	12	13	2
7	20	21	1
8	14	8	2
9	17	20	2
10	16	10	2

-5 10 1

4	31	29	1
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6	18	14	2
7	33	31	1
8	18	19	2

-4 1 1

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3	146	142	1
4	133	136	1
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6	22	25	1
7	27	27	1
8	282	283	2
9	70	68	1
10	14	10	2
11	35	32	1
12	-8	2	3

-4 2 1

1	245	234	2
2	137	129	1
3	46	40	0
4	137	132	1
5	61	62	0
6	92	87	1
7	119	117	1

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8	120	121	1
9	45	45	1
10	47	48	1
11	-8	3	2
12	36	33	1

-4 3 1

1	11	9	1
2	102	102	1
3	37	37	0
4	36	36	0
5	252	255	2
6	196	196	1
7	47	43	1
8	23	20	1
9	29	31	1
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11	50	49	1
12	26	23	1

-4 4 1

1	58	62	0
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3	103	103	1
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5	76	78	1
6	341	343	3
7	264	266	2
8	96	99	1
9	34	35	1
10	49	47	1
11	13	9	2
12	23	21	1

-4 5 1

1	64	65	1
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3	18	19	1
4	74	73	1
5	48	52	1
6	62	58	1
7	105	106	1
8	67	69	1
9	69	69	1
10	49	52	1
11	67	65	1
12	13	4	2

-4 6 1

1	27	27	1
2	37	39	1
3	151	149	1
4	36	36	1
5	112	113	1
6	98	98	1
7	99	102	1
8	65	68	1
9	66	68	1
10	24	21	1
11	89	85	1
12	51	47	1

-4 7 1

1	59	59	1
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3	70	70	1
4	42	40	1
5	118	119	1
6	115	118	1
7	52	52	1
8	31	34	1
9	11	7	2
10	28	32	1
11	56	50	1
12	32	36	1

-4 8 1

1	10	15	2
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4	28	29	1
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6	10	4	2
7	11	7	2
8	55	55	1
9	36	34	1
10	28	24	1
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-4 9 1

1	53	48	1
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4	46	44	1
5	27	25	1
6	-12	3	1
7	48	50	1
8	13	14	2
9	27	25	1
10	67	63	1
11	72	69	1

-4 10 1

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4	18	20	2
5	16	10	2
6	-9	2	2
7	16	21	2
8	33	33	1
9	-7	7	3

-3 1 1

1	210	206	1
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3	21	13	0
4	80	71	0
5	224	215	2
6	139	138	1
7	15	11	1
8	71	71	1
9	48	50	1
10	10	3	2
11	11	3	2
12	17	18	2

-3 2 1

1	31	31	0
2	129	130	1
3	66	66	0
4	70	71	0
5	26	27	0
6	106	104	1
7	396	401	3
8	146	146	1
9	85	86	1
10	43	41	1
11	23	23	1
12	9	3	3

-3 3 1

1	291	290	2
2	94	92	1
3	275	281	2
4	108	111	1
5	107	106	1
6	121	118	1
7	299	297	2
8	224	224	2
9	21	22	1
10	-3	3	4
11	-8	3	3
12	22	20	1

-3 4 1

1	57	57	0
2	155	155	1
3	127	123	1
4	92	94	1
5	40	37	0
6	61	62	1
7	100	102	1
8	64	63	1
9	97	97	1
10	71	71	1
11	6	11	3
12	25	18	1

-3 5 1

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6	186	183	1
7	103	105	1
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9	49	51	1
10	29	29	1
11	9	20	2
12	105	97	1
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-3 6 1

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3	18	20	1
4	32	34	1
5	91	90	1
6	55	55	1
7	14	13	1
8	-8	8	2
9	37	39	1
10	21	19	1
11	12	17	2
12	33	27	1
13	-6	7	4

-3 7 1

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5	18	14	1
6	64	64	1
7	46	45	1
8	60	61	1
9	79	78	1
10	11	15	2
11	82	77	1
12	95	91	1

-3 8 1

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5	35	37	1
6	89	87	1
7	41	41	1
8	87	93	1
9	44	51	1
10	67	62	1
11	50	47	1
12	18	15	2

-3 9 1

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6	9	7	2
7	7	9	3
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-3 10 1

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7	31	31	1
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11	60	56	1

-3 11 1

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5	13	8	2
6	64	63	1
7	-12	5	2
8	32	30	1
9	28	29	1

-2 1 1

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3	150	147	1
4	235	239	2
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6	26	20	1
7	55	53	1
8	318	317	2
9	87	90	1
10	42	45	1
11	17	12	2
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-2 2 1

1	266	261	2
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3	409	399	3
4	300	295	2
5	5	0	2
6	222	226	2
7	117	119	1
8	102	98	1
9	101	101	1
10	27	30	1
11	38	39	1
12	21	20	1

-2 3 1

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3	52	51	0
4	-3	3	2
5	285	282	2
6	232	225	2
7	118	118	1
8	91	93	1
9	43	44	1
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11	16	17	2
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-2 4 l

1	12	13	1
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3	195	203	1
4	81	79	1
5	44	50	0
6	194	203	1
7	126	125	1
8	8	1	2
9	28	27	1
10	38	40	1
11	45	43	1
12	38	37	1
13	42	36	1

-2 5 l

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3	70	63	0
4	166	164	1
5	53	54	0
6	85	83	1
7	51	48	1
8	43	42	1
9	8	2	2
10	46	46	1
11	8	8	3
12	54	48	1
13	73	70	1

-2 6 l

1	5	0	3
2	48	49	1
3	267	264	2
4	51	52	0
5	62	63	1
6	81	79	1
7	18	9	1
8	108	109	1
9	85	87	1
10	13	21	2
11	59	57	1
12	78	74	1
13	50	45	1

-2 7 l

1	9	11	2
2	127	130	1
3	108	108	1
4	38	36	1
5	81	80	1
6	36	36	1
7	179	181	1
8	50	50	1
9	24	33	1
10	94	100	1
11	14	14	2
12	17	17	2
13	44	45	1

-2 8 l

1	34	34	1
2	68	65	1
3	80	79	1
4	26	27	1
5	65	67	1
6	34	37	1
7	60	59	1
8	8	10	2
9	24	23	1
10	-6	1	3
11	31	29	1
12	44	39	1

-2 9 l

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3	10	8	2
4	38	35	1
5	10	0	2
6	2	6	5
7	125	129	1
8	40	39	1
9	43	43	1
10	47	47	1
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12	7	12	3

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1	33	30	1
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3	42	39	1
4	25	25	1
5	57	57	1
6	19	21	1
7	60	64	1
8	9	16	3
9	30	30	1
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11	12	13	2

-2 11 l

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6	30	29	1
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8	22	23	1
9	31	29	1
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-1 1 l

1	402	421	3
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3	506	507	4
4	348	337	3
5	75	77	0
6	83	85	1
7	21	18	1
8	22	18	1
9	54	55	1
10	11	11	2
11	32	32	1
12	-12	9	2

-1 2 l

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5	28	27	0
6	156	150	1
7	249	246	2
8	52	55	1
9	32	30	1
10	25	22	1
11	24	29	1
12	19	19	2

-1 3 l

1	22	25	0
2	289	285	2
3	98	93	1
4	99	98	1
5	170	176	1
6	60	65	0
7	34	37	0
8	61	61	1
9	64	63	1
10	-11	0	1
11	63	60	1
12	28	25	1
13	6	0	4

-1 4 l

1	164	166	1
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3	9	10	1
4	478	462	4
5	161	164	1
6	47	41	0
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8	18	17	1
9	71	73	1
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11	23	23	1
12	26	26	1
13	53	48	1

-1 5 l

1	40	41	0
2	22	22	0
3	110	103	1
4	232	224	2
5	117	124	1
6	110	109	1
7	33	33	1
8	179	178	1
9	93	93	1
10	44	49	1
11	107	111	1
12	56	53	1
13	22	18	1

-1 6 l

1	47	45	0
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4	319	319	2
5	10	8	1
6	41	43	1
7	80	82	1
8	63	67	1
9	19	19	1
10	67	63	1
11	58	64	1
12	34	34	1
13	31	26	1

-1 7 l

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3	116	117	1
4	75	73	1
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6	93	96	1
7	4	6	3
8	126	131	1
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10	57	57	1
11	56	56	1
12	-11	3	2
13	18	12	2

-1 8 l

1	45	46	1
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3	59	57	1
4	75	74	1
5	10	14	2
6	66	67	1
7	15	16	1
8	121	129	1
9	41	42	1
10	67	69	1
11	17	21	1
12	30	31	1
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-1 9 l

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5	98	96	1
6	70	73	1
7	2	4	5
8	5	4	3
9	7	13	3
10	43	40	1
11	42	40	1
12	13	15	2

-1 10 l

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3	11	6	2
4	11	13	2
5	33	35	1
6	76	75	1
7	56	56	1
8	29	26	1
9	32	33	1
10	23	27	1
11	-9	9	2
12	66	64	1

-1 11 l

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3	25	27	1
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6	70	72	1
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9	31	29	1
10	47	47	1
11	83	74	1

-1 12 l

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7	-10	0	2
8	8	4	3
9	32	32	1

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Diethylamino-II-Thiobarbituric Acid

0 0 1

1	359	356	3
2	298	307	2
3	178	180	1
4	39	41	0
5	11	8	1
6	106	108	1
7	95	94	1
8	109	108	1
9	30	31	1
10	39	39	1
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0 1 1

-11	24	24	1
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-2	85	81	0
-1	71	68	0
0	376	380	3
1	389	405	3
2	112	111	1
3	136	128	1
4	92	88	0
5	95	93	1
6	166	169	1
7	-11	1	1
8	110	109	1
9	29	24	1
10	45	44	1
11	-6	7	3
12	28	23	1

0 2 1

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-7	25	18	1
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-1	552	554	4
0	506	519	4
1	120	123	1
2	109	116	1
3	56	54	0
4	359	353	3
5	328	316	2
6	152	155	1
7	65	63	1
8	62	61	1
9	76	75	1
10	-3	6	4
11	18	14	1
12	20	15	1

0 3 1

-9	10	9	2
-8	43	46	1
-7	35	31	1
-6	12	9	2
-5	65	63	1
-4	20	20	1
-3	204	201	1
-2	375	379	3
-1	254	251	2

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3	82	80	0
4	54	52	0
5	521	490	4
6	72	75	0
7	13	16	1
8	15	16	1
9	59	59	1
10	87	89	1
11	13	16	2
12	28	30	1
13	16	15	2

0 4 1

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2	152	155	1
3	83	78	0
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6	13	19	1
7	13	8	1
8	159	160	1
9	175	176	1
10	6	9	3
11	-8	10	2
12	67	70	1
13	8	5	3

0 5 1

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1	147	151	1
2	78	79	0
3	298	292	2
4	362	357	3
5	231	219	2
6	103	108	1
7	214	215	2
8	-6	7	2
9	97	95	1
10	22	24	1
11	32	28	1
12	5	6	4
13	23	24	1

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1	43	44	0
2	15	16	1

3	66	65	0
4	54	54	0
5	28	27	0
6	10	6	1
7	42	40	1
8	57	60	1
9	132	143	1
10	30	36	1
11	67	64	1
12	14	16	2
13	40	42	1

0 7 1

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-2	16	14	1
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7	118	119	1
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9	37	49	1
10	55	56	1
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12	20	21	1
13	17	17	2

0 8 1

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8	80	79	1
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10	54	56	1
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12	19	20	1
13	42	43	1

0 9 1

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4	32	35	1
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6	39	37	1
7	124	129	1
8	9	16	2
9	65	63	1
10	-11	0	2
11	37	39	1
12	59	58	1
13	25	27	1

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-2	-1	2	7
-1	9	9	3
0	7	13	3
1	-6	2	3
2	39	41	1
3	10	9	2
4	18	18	1
5	32	32	1
6	63	60	1
7	15	20	1
8	41	40	1
9	52	55	1
10	68	67	1
11	72	74	1
12	35	34	1

0 11 1

0	-11	0	2
1	14	10	2
2	15	16	2
3	11	3	2
4	73	72	1
5	28	23	1
6	65	66	1
7	40	43	1
8	24	22	1
9	9	10	3
10	35	33	1
11	4	3	5

0 12 1

3	53	51	1
4	59	58	1
5	36	32	1
6	10	13	3
7	11	13	2
8	12	17	2
9	9	9	3
10	84	75	1

1 -10 1

0	-9	8	2
1	-12	4	2

1 -9 1

0	31	23	1
1	14	10	2
2	7	10	3
3	7	5	3

1 -8 1

0	-2	0	4
1	14	11	2
2	13	18	2
3	6	6	4
4	13	12	2

1 -7 1

0	24	30	1
1	16	15	1
2	36	33	1
3	31	32	1
4	24	23	1
5	13	8	2

1 -6 1

0	60	58	1
1	15	10	1
2	72	70	1
3	29	24	1
4	10	3	2

5	20	19	1	-3	137	136	1	-3	162	161	1	1	14	13	1
6	43	43	1	-2	344	337	2	-2	104	103	1	2	99	96	1
				-1	346	362	2	-1	209	213	1	3	94	96	1
1	-5	1		0	102	94	0	0	194	191	1	4	160	155	1
				1	196	199	1	1	38	40	0	5	62	57	0
0	45	46	0	2	306	302	2	2	133	137	1	6	102	106	1
1	14	1	1	3	41	39	0	3	9	3	1	7	171	178	1
2	142	146	1	4	129	131	1	4	309	292	2	8	40	39	1
3	52	56	1	5	160	159	1	5	612	603	5	9	63	65	1
4	32	28	1	6	79	75	1	6	267	255	2	10	16	24	1
5	19	27	1	7	122	124	1	7	83	88	1	11	35	40	1
6	13	11	2	8	35	33	1	8	51	57	1	12	59	59	1
7	14	15	2	9	18	13	1	9	70	73	1	13	24	23	1
				10	47	43	1	10	21	28	1				
1	-4	1		11	-7	8	3	11	36	35	1	1	7	1	
								12	5	3	4				
0	244	242	2	1	1	1						-6	-8	7	3
1	388	385	3					1	4	1		-5	35	30	1
2	232	229	2	-11	10	10	3					-4	33	32	1
3	157	162	1	-10	15	7	2	-9	14	6	2	-3	15	16	1
4	205	201	1	-9	173	176	1	-8	18	11	1	-2	70	71	1
5	5	0	3	-8	34	29	1	-7	28	32	1	-1	79	77	1
6	36	34	1	-7	43	44	1	-6	10	11	2	0	189	191	1
7	18	18	1	-6	8	9	2	-5	107	106	1	1	93	93	1
8	-4	0	4	-5	15	15	1	-4	73	68	1	2	168	169	1
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				-2	588	596	5	-1	189	187	1	5	13	17	1
0	242	233	2	-1	692	711	5	0	122	120	1	6	73	75	1
1	42	41	0	0	282	292	2	1	144	142	1	7	34	35	1
2	134	130	1	1	473	482	4	2	158	152	1	8	181	191	1
3	174	170	1	2	92	100	0	3	53	52	0	9	49	53	1
4	88	87	1	3	91	84	0	4	460	441	3	10	20	22	1
5	53	56	1	4	260	262	2	5	90	84	1	11	37	36	1
6	47	46	1	5	280	277	2	6	-2	16	3	12	17	13	2
7	3	3	4	6	366	362	3	7	124	132	1	13	34	35	1
8	27	20	1	7	33	32	1	8	129	130	1				
9	-5	7	4	8	48	46	1	9	65	65	1	1	8	1	
				9	6	9	3	10	107	109	1				
1	-2	1		10	25	24	1	11	45	45	1	-5	9	6	3
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0	421	427	3	12	-9	7	3	13	23	19	1	-3	13	11	2
1	1082	1070	9									-2	18	12	1
2	55	53	0	1	2	1		1	5	1		-1	12	13	2
3	119	117	1									0	32	35	1
4	123	122	1	-10	37	34	1	-8	9	12	3	1	18	16	1
5	35	37	1	-9	17	14	1	-7	18	15	1	2	8	10	2
6	13	19	1	-8	57	56	1	-6	16	19	1	3	4	3	3
7	27	21	1	-7	110	110	1	-5	66	69	1	4	25	25	1
8	15	16	2	-6	-3	7	3	-4	47	42	1	5	31	32	1
9	26	20	1	-5	123	121	1	-3	70	71	1	6	220	223	2
10	13	11	2	-4	33	29	0	-2	35	30	1	7	64	66	1
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1	-1	1		-2	67	68	0	0	188	195	1	9	47	44	1
				-1	488	501	4	1	68	67	0	10	9	22	2
0	255	243	2	0	313	321	2	2	33	36	0	11	79	81	1
1	1480	1446	12	1	214	206	1	3	122	123	1	12	103	102	1
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3	91	93	1	3	95	92	0	5	74	81	0				
4	114	114	1	4	75	77	0	6	27	26	0	1	9	1	
5	127	127	1	5	102	103	1	7	85	82	1				
6	93	92	1	6	204	194	1	8	87	89	1	-4	8	9	3
7	60	60	1	7	136	138	1	9	2	5	4	-3	25	17	1
8	63	64	1	8	16	15	1	10	56	66	1	-2	57	55	1
9	75	76	1	9	26	28	1	11	48	48	1	-1	40	44	1
10	16	12	2	10	55	57	1	12	-1	1	6	0	29	31	1
11	-10	1	2	11	23	27	1	13	22	24	1	1	22	22	1
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1	0	1						1	6	1		3	14	13	1
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2	19	18	1
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5	106	109	1
6	123	120	1
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8	12	18	2
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11	34	33	1
12	40	42	1

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6	2	5	5
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8	38	35	1
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6	50	49	1
7	15	13	2
8	32	28	1
9	51	50	1
10	-8	4	3

1 13 1

6	13	9	2
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8	32	29	1

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2 -9 1

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1	9	1	3
2	5	4	4

2 -8 1

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3	33	32	1
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2 -7 1

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2 -6 1

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2 -5 1

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1	130	125	1
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4	63	70	1
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6	36	36	1
7	7	5	3

2 -4 1

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3	17	11	1
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6	5	7	3
7	3	3	5
8	18	17	2

2 -3 1

0	218	213	1
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2	758	760	6
3	76	75	1
4	78	79	1
5	39	42	1
6	24	21	1
7	22	19	1
8	26	25	1
9	-9	7	3

2 -2 1

0	200	204	1
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2	169	164	1
3	87	88	1
4	73	73	1
5	18	22	1
6	23	23	1
7	-5	1	3
8	20	19	1
9	32	31	1
10	20	26	2

2 -1 1

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2	218	212	1
3	89	90	1
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1	314	318	2
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3	23	24	0
4	121	123	1
5	142	139	1
6	29	25	1
7	110	114	1
8	58	55	1
9	2	7	5
10	11	12	2
11	39	35	1

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-3	172	165	1
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-1	173	171	1
0	94	94	0
1	49	53	0
2	434	435	3
3	129	129	1
4	141	149	1
5	111	108	1
6	178	178	1
7	17	22	1
8	32	34	1
9	39	40	1
10	45	45	1
11	20	26	1

2 2 1

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1	46	42	0
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4	69	69	0
5	300	287	2
6	256	250	2
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1	404	413	3
2	324	322	2
3	448	451	3
4	171	169	1
5	150	142	1
6	99	104	1
7	55	60	0
8	28	27	1
9	32	34	1
10	55	53	1
11	52	53	1
12	53	49	1

2 4 1

-9	23	19	1
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-7	14	9	2
-6	26	28	1
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-3	74	71	1
-2	40	37	0
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1	13	12	1
2	169	162	1
3	106	112	1
4	153	152	1
5	247	249	2
6	24	27	0
7	30	30	1
8	107	111	1
9	-8	7	2
10	57	51	1
11	35	38	1
12	10	9	2
13	32	30	1

2 5 1

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-7	19	20	1
-6	34	32	1
-5	72	69	1
-4	5	6	3
-3	26	26	1
-2	124	127	1
-1	60	62	0
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1	205	198	1
2	241	239	2
3	121	127	1
4	179	182	1
5	1	5	4
6	10	8	1
7	98	99	1
8	23	25	1
9	76	79	1
10	38	38	1
11	36	34	1
12	60	58	1
13	31	30	1

2 6 1

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-7	14	14	2
-6	46	50	1
-5	67	66	1
-4	50	47	1
-3	48	44	1
-2	33	34	1
-1	164	162	1
0	6	1	2
1	146	144	1
2	219	219	2
3	188	192	1
4	95	95	1
5	255	254	2
6	40	42	0
7	120	121	1
8	25	26	1
9	165	173	1
10	52	49	1
11	47	44	1
12	18	22	1
13	42	41	1

2 7 1

-6	-3	12	5
-5	44	38	1
-4	14	14	2
-3	22	22	1
-2	44	40	1
-1	92	90	1
0	10	4	2
1	30	30	1
2	80	81	1
3	86	88	1
4	14	13	1
5	75	75	1
6	-6	0	2
7	77	78	1
8	156	159	1
9	-9	10	2
10	32	28	1
11	96	103	1
12	81	80	1
13	54	51	1

2 8 1

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-3	-9	1	2
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2	12	12	1
3	67	69	1
4	98	99	1
5	116	117	1
6	104	107	1
7	172	174	1
8	107	110	1
9	-8	1	2
10	79	81	1
11	25	23	1
12	10	0	2
13	52	53	1

2 9 1

-4	-9	4	3
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-2	21	25	1
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1	6	12	3
2	83	85	1
3	29	28	1
4	89	91	1

5	137	134	1
6	147	145	1
7	149	152	1
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9	45	43	1
10	26	27	1
11	40	43	1
12	72	69	1
13	15	7	2

2 10 1

-2	40	38	1
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1	24	20	1
2	-1	4	5
3	57	59	1
4	181	180	1
5	186	185	1
6	15	15	1
7	89	87	1
8	-9	7	2
9	37	37	1
10	43	42	1
11	27	26	1
12	11	5	2

2 11 1

-1	2	6	6
0	15	19	2
1	27	25	1
2	59	55	1
3	32	36	1
4	114	111	1
5	33	34	1
6	8	0	3
7	-6	8	3
8	56	54	1
9	43	43	1
10	25	30	1
11	41	45	1
12	60	57	1

2 12 1

1	6	6	4
2	17	14	2
3	104	108	1
4	44	44	1
5	29	26	1
6	-7	11	3
7	9	11	3
8	20	19	1
9	-3	12	5
10	71	61	1
11	60	57	1

2 13 1

4	77	75	1
5	28	28	1
6	7	11	4
7	-3	2	5
8	24	22	1
9	35	36	1

3 -9 1

0	14	13	2
1	-7	3	3

3 -8 1

0	30	30	1
1	11	8	2
2	24	25	1

3	15	18	2

3 -7 1

0	18	12	1
1	-6	5	3
2	69	65	1
3	76	77	1
4	54	57	1

3 -6 1

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2	11	11	2
3	15	15	1
4	28	34	1
5	29	29	1

3 -5 1

0	44	44	1
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2	129	132	1
3	150	156	1
4	30	33	1
5	23	16	1
6	0	8	7
7	22	21	1

3 -4 1

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2	76	78	1
3	268	282	2
4	65	64	1
5	42	45	1
6	2	5	5
7	21	18	1
8	9	6	3

3 -3 1

0	242	242	2
1	73	69	0
2	75	74	1
3	67	62	1
4	9	3	2
5	3	8	4
6	-5	3	3
7	46	44	1
8	24	28	1

3 -2 1

0	260	251	2
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2	20	16	1
3	71	69	1
4	26	28	1
5	51	47	1
6	85	80	1
7	88	93	1
8	60	65	1
9	13	9	2

3 -1 1

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1	228	228	2
2	170	180	1
3	31	29	0
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5	8	11	2
6	11	8	1
7	72	72	1
8	7	11	3

9	37	36	1
10	27	24	1

3 0 1

-11	23	18	1
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-9	203	205	2
-8	127	126	1
-7	174	176	1
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-5	111	111	1
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-3	253	241	1
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1	246	255	2
2	100	96	1
3	76	77	0
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5	30	29	1
6	134	137	1
7	143	147	1
8	20	20	1
9	17	18	1
10	7	11	3
11	5	15	4

3 1 1

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3	143	145	1
4	134	135	1
5	94	98	1
6	110	111	1
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8	23	23	1
9	57	61	1
10	8	16	3
11	17	22	2

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2	285	283	2
3	304	307	2
4	197	195	1
5	43	43	0
6	161	158	1
7	68	63	1
8	-6	8	2
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10	36	37	1

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Diethylamino-II-Thiobarbituric Acid

11 12 9 2
12 25 23 1

3 3 1

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1	73	73	0
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3	22	25	0
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9	40	43	1
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3 4 1

-9	24	26	1
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2	416	396	3
3	358	353	3
4	120	120	1
5	36	40	0
6	144	148	1
7	23	27	1
8	-1	4	5
9	114	115	1
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11	15	15	2
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3 5 1

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3	83	81	0
4	58	58	0
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6	87	90	1
7	77	76	1
8	195	197	1
9	66	65	1
10	90	92	1
11	50	48	1
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3 6 1

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6	218	217	2
7	5	9	2
8	147	150	1
9	168	166	1
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11	25	24	1
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3 7 1

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3 8 1

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3	97	97	1
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6	276	275	2
7	165	166	1
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9	63	65	1
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12	28	28	1
13	18	15	2

3 9 1

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3	36	35	1
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6	89	89	1
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8	96	98	1
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11	50	51	1
12	35	38	1
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3	72	70	1
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8	92	91	1
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11	36	33	1
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3 11 1

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1	7	10	3
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3	18	16	1
4	165	162	1
5	117	119	1
6	52	54	1
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8	12	8	2
9	63	63	1
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11	70	58	1
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3 12 1

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4 -4 1

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4 -3 1

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3	121	124	1
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4 -2 1

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4 2 1

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4 3 1

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4 4 1

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4 5 1

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4 6 1

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5 -7 1

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-3	29	30	1
-2	78	80	1
-1	179	178	1
0	230	236	2
1	108	108	1
2	14	13	1
3	44	45	1
4	65	69	1
5	83	85	1
6	27	30	1
7	-1	5	6
8	60	58	1
9	17	20	2

9 5 1

-7	4	4	5
-6	16	17	2
-5	37	37	1
-4	23	23	1
-3	41	36	1
-2	40	42	1
-1	76	78	1
0	54	56	1
1	-4	2	3
2	91	97	1
3	5	12	3
4	50	52	1
5	9	7	2
6	17	17	1
7	19	26	1
8	25	23	1
9	81	78	1
10	10	9	3

9 6 1

-6	30	30	1
-5	9	4	3
-4	46	40	1
-3	37	38	1
-2	93	97	1
-1	20	21	1
0	47	52	1
1	87	84	1
2	62	59	1
3	55	64	1
4	130	138	1
5	121	126	1
6	8	11	2
7	13	12	2
8	64	58	1
9	6	6	3
10	7	9	3

9 7 1

-5	12	15	2
-4	23	18	1
-3	15	16	2
-2	53	56	1
-1	46	45	1
0	51	50	1
1	-5	3	3
2	14	18	1
3	99	96	1
4	62	64	1
5	92	102	1
6	110	112	1
7	10	4	2
8	13	13	2
9	51	51	1
10	12	14	2

9 8 1

-4	12	5	2
-3	22	20	1
-2	1	6	6
-1	-4	0	4
0	-8	7	2
1	57	55	1
2	24	20	1

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3	74	80	1	3	22	24	1	3	23	24	1	9	20	20	2
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5	-8	0	2	10	-1	1		5	27	22	1	10	8	1	
6	38	40	1					6	43	41	1				
7	35	30	1	0	51	49	1	7	-2	4	6	-3	60	58	1
8	49	51	1	1	49	48	1	8	-11	3	2	-2	36	34	1
9	-11	5	2	2	29	27	1					-1	36	33	1
10	14	16	2	3	34	31	1	10	4	1		0	16	19	2
				4	33	27	1					1	7	13	3
9	9	1		5	5	4	4	-7	52	56	1	2	46	45	1
								-6	27	24	1	3	47	42	1
-3	14	17	2	10	0	1		-5	22	23	1	4	27	35	1
-2	-7	4	3					-4	-6	0	3	5	-7	12	3
-1	-11	2	2	-8	37	33	1	-3	51	47	1	6	19	17	1
0	23	21	1	-7	7	4	3	-2	67	66	1	7	33	31	1
1	13	10	2	-6	17	16	2	-1	42	42	1	8	-5	1	4
2	17	7	1	-5	26	27	1	0	18	21	1	9	38	36	1
3	83	93	1	-4	20	21	1	1	48	51	1				
4	69	72	1	-3	25	23	1	2	45	42	1	10	9	1	
5	-8	2	2	-2	42	40	1	3	60	64	1				
6	81	79	1	-1	21	25	1	4	26	23	1	-2	15	13	2
7	2	8	5	0	92	92	1	5	84	86	1	-1	69	68	1
8	-10	4	2	1	146	146	1	6	54	53	1	0	44	42	1
9	-12	4	2	2	84	85	1	7	11	12	2	1	50	50	1
10	37	31	1	3	19	17	1	8	18	17	2	2	43	43	1
				4	63	57	1					3	30	28	1
9	10	1		5	45	46	1	10	5	1		4	6	8	3
				6	15	17	2					5	-1	4	6
-1	30	28	1					-6	15	14	2	6	12	14	2
0	24	21	1	10	1	1		-5	16	18	2	7	67	65	1
1	39	35	1					-4	14	15	2	8	19	19	2
2	68	63	1	-8	33	33	1	-3	19	16	1	9	38	32	1
3	44	49	1	-7	18	20	2	-2	17	14	1				
4	-8	3	2	-6	1	9	6	-1	112	113	1	10	10	1	
5	11	8	2	-5	3	4	4	0	42	45	1				
6	17	19	1	-4	98	98	1	1	-5	2	3	-1	1	10	7
7	-5	12	4	-3	28	30	1	2	22	21	1	0	9	5	3
8	65	61	1	-2	-3	4	4	3	31	32	1	1	43	40	1
9	19	16	2	-1	20	20	1	4	105	106	1	2	-3	1	5
10	76	65	1	0	28	24	1	5	97	98	1	3	7	13	3
				1	63	62	1	6	70	73	1	4	-8	5	3
9	11	1		2	73	73	1	7	58	56	1	5	27	24	1
				3	25	22	1	8	5	0	4	6	35	31	1
0	3	10	5	4	-1	0	6	9	31	28	1	7	26	27	1
1	6	4	4	5	11	16	2					8	41	38	1
2	17	21	2	6	9	5	3	10	6	1		9	-4	17	5
3	38	35	1												
4	18	18	2	10	2	1		-5	37	35	1	10	11	1	
5	37	35	1					-4	56	52	1				
6	36	36	1	-8	54	49	1	-3	44	38	1	1	16	14	2
7	6	10	3	-7	26	26	1	-2	13	10	2	2	-8	0	3
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3	9	9	3	-1	71	71	1	4	18	12	1	8	79	66	1
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6	30	32	1	2	84	84	1	7	53	52	1				
7	68	60	1	3	37	37	1	8	17	18	2	0	17	15	2
8	13	8	2	4	32	29	1	9	28	26	1				
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10	-4	1		6	41	36	1	10	7	1					
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				-7	-6	8	3	-1	13	16	2	11	-1	1	
0	22	16	1	-6	17	18	2	0	9	10	2				
1	24	21	1	-5	38	39	1	1	4	12	4	0	20	19	1
2	46	40	1	-4	6	6	3	2	21	20	1	1	41	37	1
				-3	28	30	1	3	6	3	3	2	63	61	1
10	-2	1		-2	39	37	1	4	101	103	1	3	33	34	1
				-1	21	19	1	5	5	5	3				
0	16	15	2	0	116	115	1	6	23	23	1	11	0	1	
1	61	57	1	1	93	92	1	7	76	73	1				
2	44	41	1	2	69	70	1	8	11	8	2	-7	66	61	1

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-6	12	14	2					1	37	36	1	5	-9	3	3
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0	21	23	1	-2	14	8	2	7	24	26	1	-3	8	1	3
1	61	57	1	-1	4	8	4					-2	12	15	2
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3	32	33	1	1	41	42	1					0	63	63	1
4	40	36	1	2	32	28	1	4	30	27	1	1	25	20	1
				3	67	67	1	5	23	18	1	2	17	14	2
11	1	1		4	24	21	1					3	21	24	1
				5	43	42	1	12	-1	1		4	37	37	1
-7	28	25	1	6	21	19	1					5	-3	2	5
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-4	23	27	1					12	0	1		12	6	1	
-3	24	23	1	11	6	1									
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-1	17	16	1	-4	11	5	2	-4	19	20	2	-2	19	20	2
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3	64	64	1	0	7	0	3	0	13	6	2	2	-8	5	2
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-4	30	26	1					-2	31	29	1	-1	32	30	1
-3	-8	4	2	11	7	1		-1	40	40	1	0	45	40	1
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1	17	20	1	-1	42	40	1	3	22	19	1	4	-7	3	3
2	12	6	2	0	62	58	1					5	15	15	2
3	16	13	2	1	4	9	4	12	2	1		6	9	9	3
4	8	1	3	2	37	41	1								
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6	34	29	1	4	45	41	1	-4	28	26	1				
				5	16	12	2	-3	10	8	2	-1	14	11	2
11	3	1		6	2	7	5	-2	12	3	2	0	29	26	1
				7	9	7	3	-1	26	24	1	1	43	41	1
-6	23	27	1	8	24	22	1	0	7	7	3	2	-9	2	2
-5	38	37	1					1	30	33	1	3	25	21	1
-4	9	18	2	11	8	1		2	41	39	1	4	28	24	1
-3	29	27	1					3	22	19	1	5	35	37	1
-2	71	70	1	-2	45	42	1	4	-11	5	2	6	34	32	1
-1	30	34	1	-1	1	4	6								
0	39	42	1	0	36	36	1	12	3	1		12	9	1	
1	30	30	1	1	16	19	2								
2	34	36	1	2	9	12	2	-5	30	28	1	1	23	19	1
3	45	44	1	3	11	11	2	-4	17	18	2	2	41	38	1
4	11	16	2	4	25	27	1	-3	42	38	1	3	21	22	1
5	36	38	1	5	28	27	1	-2	44	42	1	4	8	3	3
6	50	50	1	6	2	7	6	-1	23	16	1	5	12	11	2
7	27	27	1	7	18	16	2	0	18	17	1	6	22	17	1
				8	23	24	1	1	26	25	1				
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				11	9	1		3	-4	1	4				
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-1	11	16	2	3	-14	3	1	-4	23	24	1				
0	29	31	1	4	18	20	1	-3	47	44	1	-3	31	26	1
1	86	86	1	5	54	50	1	-2	26	22	1	-2	63	57	1
2	23	17	1	6	-11	1	2	-1	51	53	1	-1	27	23	1
3	29	27	1	7	8	9	3	0	10	7	2	0	11	5	2
4	14	9	2	8	65	63	1	1	20	18	1	1	3	3	5
5	57	55	1					2	10	1	2	2	12	14	2
6	15	19	2	11	10	1		3	18	13	2				
7	20	25	2					4	21	20	1	13	3	1	

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Diethylamino-II-Thiobarbituric Acid

-3	37	35	1
-2	13	9	2
-1	12	5	2
0	57	55	1
1	19	17	2
2	7	4	3
3	9	7	3

13 4 1

-2	8	4	3
-1	12	9	2
0	39	41	1
1	49	48	1
2	18	14	2
3	-5	5	4

13 5 1

-2	14	13	2
-1	19	18	2
0	32	28	1
1	18	16	2
2	26	26	1
3	13	14	2
4	9	13	3

13 6 1

-1	-2	6	6
0	6	3	4
1	58	53	1
2	43	43	1
3	-9	6	3
4	41	36	1

13 7 1

0	-6	5	4
1	-4	1	5
2	49	45	1
3	24	24	1
4	17	21	2

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